What is the bond order for N2+?

See Quora: What is the bond order for N2+? https://qr.ae/TUtkVn

The MO method for N2+ gives the bond order equal to 2.5.

But first, we look at the diagram of molecular orbitals for N2 (the bond order for the nitrogen molecule is 3).

Let's remember that the order of bond by the MO method is:

bond order = (number of electrons in binding orbitals - number of electrons in disintegrating orbitals) / 2

From the diagram it is clear that for a nitrogen molecule we have a bond order equal to 3:

bond order (N2) = (10 - 4)/2 = 3

In order to calculate the bond order for N2+ it is necessary to remove one electron from the highest occupied orbital (binding) of Ϭ2px (N2 molecule), since it is this electron that has the maximum energy and therefore will have the minimum ionization energy (let's make this mental transition from the N2 molecule to the N2+ molecule).

Then, for the bond order of the N2 + molecule, we obtain:

bond order (N2+) = (9 - 4)/2 = 2.5

That is, the bond order for N2+ is 2.5.

But it is precisely this value of the order of the relation (2.5) for N2+ that is incorrect and indicates the erroneous predictions of the MO method. This becomes clear if we recall the distance between nitrogen atoms at different values of the bond order (see page 8 http://vixra.org/pdf/1606.0149v2.pdf (A short analysis of chemical bonds)):

bond order = 1, L (N – N) = 1.453 Å

bond order = 2, L (N – N) = 1.2300 Å

bond order = 3, L (N – N) = 1.0976 Å (for nitrogen molecule)

bond order = 2.5, L (N – N) = 1.157 Å, (prediction)

For the N2+ molecule, we have a distance equal to L(N – N) = 1.116 Å (see page 9 reference http://vixra.org/pdf/1606.0149v2.pdf (A short analysis of chemical bonds)), which is very close to the distance between the nitrogen atoms in the N2 molecule (L(N – N) = 1.0976 Å). Compare more approximate values: 1.12 Å (N2+) and 1.10 Å (N2), which almost coincide.

If we have the bond order 2, then the distance between the nitrogen is 1.23 Å, from where it is obvious (comparison with 1.10 Å for bond order 3), that with the bond order 2.5, the distance should be greater than 1.12 Å (according to our calculations from the multiplicity equation equal to 1.157 Å, or a more approximate value of 1.16 Å).

In order to obtain a more accurate value of the coupling ratio in the N2 + molecule, we use the corresponding equation to determine the multiplicity:

$$\text{Multiplicity (N-N)} = 0.96407492 - \frac{6.68791795}{L} + \frac{9.79339013}{L^2}$$

Whence we get, Multiplicity = 2.835.

(bond order (MO) = Multiplicity)

N2+, L = 1.116 Å, Multiplicity = 2.835, E = 846.001 kj/mole

$$E\text{ (N-N)} = 7067.14065437 - \frac{20274.81508318}{L} + \frac{14878.53765631}{L^2}$$

Considering the distance between nitrogen atoms in N2 and N2+ molecules (1.10 Å and 1.12 Å), the coupling ratio (or bond order) 2.835 for the N2+ molecule looks convincing, which confirms the applicability of the corresponding equations for analyzing various chemical bonds (prediction of the binding energy, multiplicity, lengths depending on the data available).

So, we can easily predict the energy of this bond (E = 846.001 kj/mole) by the length of the N-N bond in the N2+ molecule, which actually coincides with the experimental value (E = 843.26 kj/mole), which again confirms the predictive power of these equations.

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See pages 8–9, A short analysis of chemical bonds.
http://vixra.org/pdf/1606.0149v2.pdf https://dx.doi.org/10.2139/ssrn.3065253

See “Chemical Bond as the Main Problem of Modern Chemistry and Physics”.
http://vixra.org/pdf/1902.0042v1.pdf

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